



PHOTOSTABILITY OF PLASTICIZED POLYVINYL CHLORIDE MEMBRANES: A THEORETICAL STUDY

(Kestabilan Foto bagi Membran Plastik Polivinil Klorida: Satu Kajian Teori)

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Abstract

The calculation of spectral shifts in the UV-visible region, and the photostability of polyvinyl chloride membranes plasticized with 1-bromonaphthalene, dibutyl phthalate, dioctyl phthalate, *o*-nitrophenyl octyl ether and tricresyl phosphate, have been systematically investigated using the ZINDO/S method combined with stochastic molecular dynamics with the MMFF94 force field. A Langevin temperature bath was used for the thermostat and the simulation temperature was 298 K during the entire time of the simulation, which was set to 0.6 ns. These methods were employed to predict the molecular structure of the membranes. The absorption wavelengths and the HOMO and LUMO energies of membrane components are reported. In addition, the photostability of the membranes is discussed in the light of the absorption wavelength. Membranes plasticized with tricresyl phosphate and *o*-nitrophenyl octyl ether show less stability under the action of UV irradiation, as they absorb light with higher energy. Membranes plasticized with butyl and octyl esters of phthalic acid are more stable and show very similar behaviour. A membrane plasticized with 1-bromonaphthalene is likely to be the least sensitive to UV irradiation.

Keywords: polyvinyl chloride, membrane, molecular dynamics, excited state, photostability

Abstrak

Pengiraan anjakan spektra di dalam kawasan ultralembayung-cahaya nampak dan kestabilan foto bagi membran plastik polivinil klorida bersama 1-bromonafalena, dibutil ftalat, dioktil ftalat, *o*-nitrofenil oktil eter dan tricresil fosfat telah secara sistematik telah dikaji menggunakan kaedah ZINDO/S gabungan molekul dinamik stokastik bersama medan daya MMFF94. Suhu rendaman Langevin telah diguna untuk termostat dan suhu simulasi ialah 298 K bagi keseluruhan masa simulasi, iaitu di tetapkan pada 0.6 ns. Kaedah ini dibangunkan untuk meramal struktur molekul membran berkenaan. Panjang gelombang serapan dan tenaga HOMO dan LUMO membran dilapor. Tambahan lagi, kestabilan foto bagi membran di bincang dari aspek panjang gelombang serapan. Membran plastik bersama tricresil fosfat dan *o*-nitrofenil oktil eter menunjukkan kestabilan yang rendah terhadap penyinaran UV sebagaimana ia menyerap cahaya pada tenaga yang tinggi. Membran plastik bersama butil dan oktil ester asid ftalik adalah lebih stabil dan menunjukkan sifat yang sama. Membran plastik bersama 1-bromonafalena merupakan membran paling kurang sensitif terhadap penyinaran UV.

Kata kunci: polivinil klorida, membran, molekul dinamik, keadaan teruja, kestabilan foto

Introduction

Ion-selective electrodes (ISEs) with plasticized membranes are widely used in analytical chemistry [1, 2]. ISEs can also be used in environmental analysis [3] and in clinical studies [4, 5]. The main advantages of using ISEs are: